SUPREM-DSMC: A NEW SCALABLE, PARALLEL, REACTING, MULTIDIMENSIONAL DIRECT SIMULATION MONTE CARLO FLOW CODE

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ABSTRACT

An AFRL/NRL team has recently been selected to develop a scalable, parallel, reacting, multidimensional (SUPREM) Direct Simulation Monte Carlo (DSMC) code for the DoD user community under the High Performance Computing Modernization Office (HPCMO) Common High Performance Computing Software Support Initiative (CHSSI). This paper will introduce the JANNAF Exhaust Plume community to this three-year development effort and present the overall goals, schedule, and current status of this new code.

INTRODUCTION

Since being introduced by Bird[1] over 30 years ago, the basic DSMC technique has matured and evolved, and a number of codes exist today that are used on a regular basis in a variety of applications.[2-6] DSMC codes are applied most often in the gas dynamic flow regime in which the Knudsen Number (Kn) is in the range $0.01<Kn<10$, where Kn is the ratio of the gas mean free path to the characteristic length of the problem. This is a regime where the continuum assumptions inherent in the Navier-Stokes equations are invalid. The DSMC technique is a well established and reliable method for simulating such gas flows. These flows cover a very broad range of space and time scales, arising in low density gases that occur in high altitude applications and in high density gases in very small devices such as microelectromechanical systems (MEMS). However, there is no standard, fully-functional parallel DSMC code presently available to the JANNAF user community. The need for a modern, portable, scalable, documented, user-friendly and readily available DSMC code has been recognized by the DoD HPCMO, which has funded a three-year development effort to build such a code. An AFRL/NRL team has been assembled to accomplish this major task. Combining the resources and complementary expertise of these two research groups, this project began on January 1, 2000.

The goal of this effort is to develop and transition to the user community a modern, scalable DSMC code based on the integration of state-of-the-art collision models with advanced parallelization methods, gridding algorithms and data structures. While the paramount characteristics of the code will be robustness and ease of use, other goals include the following code capabilities:

- Parallel, scalable solution of CPU-intensive 3-D, unsteady flows
- Accurate representation of and resolution of highly nonequilibrium chemical and collisional processes
- Documented databases of key reaction rates and molecular constants

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- Automated grid adaptation and related capabilities to allow use by a broad range of non-expert users
- Standardized and documented code operation and software-design methodology
- Easily extendable user interface and data structures to allow enduring use and continued code enhancement and customization

These code capabilities should provide a valuable tool for analysis of a wide range of exhaust plume problems, as well as find use in microelectromechanical device development, hypersonic flight and reentry vehicle analysis, and investigation of spacecraft environments.

GENERAL DISCUSSION OF SUPREM-DSMC DEVELOPMENT

DEVELOPMENT PHILOSOPHY

Although both groups participating in this project have ongoing relevant research efforts, the SUPREM-DSMC project is not focused on advancing the state of the art, but is primarily concerned with providing a product in a reasonable time frame that is usable by a non-expert for real-world problems. This mandates that the code be robust, have internal checking capabilities, and provide the user feedback on the solution quality. Attention will be focused on lowering risk by implementation of proven computation models and techniques, with capabilities for adding new models and techniques as they are developed.

Many applications of interest introduce conflicting demands on the software suite, and potentially involve physical processes and features for which existing, validated, or robust DSMC models are not available. Several decision points involving tradeoffs and compromises are explicitly scheduled early in the program to determine what specific models and techniques to use in the various modules of the code. An additional challenge involves the need for a relatively large degree of automation (expert systems) in the code to allow use by novice users. Features such as local grid and time step adaptation, with appropriate heuristic control methods, will be an integral part of the software. It is also recognized that there will be a significant challenge in obtaining and maintaining portability and robustness with the desired level of novice-user convenience, as no such software has been demonstrated for the demanding applications of interest.

One vital additional criterion during the development of this code is that continued participation and advice of DSMC experts and the user community be sought and encouraged. An advisory group of experts in the field has already been assembled to serve as technical advisors and alpha and beta testers. The advisory board will review the technical approach during the initial phases of the project, and will periodically participate in status review and problem resolution. Technology transfer to the user community is an integral component of the project and will be accomplished through a series of meetings, training workshops and frequent dialogue between the software developers and applications experts. It is strongly desired that any interested users contact one of the team members as soon as possible.

A web site has been set up for dissemination of information to the interested technical community: http://www.lcp.nrl.navy.mil/~ckaplan/chssi.html.

QUESTIONAIRE RESULTS

One of the first actions of the SUPREM-DSMC team was to compose a questionnaire that was sent to DSMC practitioners and potential SUPREM-DSMC users to obtain information on the types of applications of interest and the required code capabilities. Most respondents were experienced DSMC users or developers. They were interested in a wide range of applications, with a majority primarily concerned with rocket exhaust plumes and reentry vehicle flow. Due to the preponderance of interest in plumes, the respondents were most interested in using DSMC simulations to obtain detailed flowfield information at steady state in complex 2-dimensional and 3-dimensional geometries with complex chemistry at elevated gas temperatures and with inert solid surfaces. They also felt that the features of

Table 1: Capabilities Timeline

Software Release	α	β	IOC
Release Date	June 2001	June 2002	Dec 2002
Geometry	2D	3D	
Grid	Fixed	Adapting	
Gas Species	Monatomic, Multispecies	Arbitrary # of Modes, Continuous/Quantized, Databases	
Collision	Elastic	Inelastic Reacting	
Boundary Conditions			
Source	Constant Freestream	Spatial Varying Time Dep.	
Wall	Fully Accom (Maxwell)	Incomplete Accommodation, Spatial Varying, Outgassing, Time Dependent Motion	
User Interface	Test File	GUI	
Automation			
Time Step	Global, Input	Local Collision Frequency, Memory Limits, Collision	
Spatial Weights	Global, Input	Separation, Local Cell Population	
Host Architecture	SP2, O2K, SP3	SP2, O2K, SP3, ES-40 (Alpha)	
Documentation	α Doc	β Doc	IOC Doc
Demos	2D Missile Body/Plume 2D Microchannel	3D Missile Body/Plume 3D Microchannel	

Hierarchical and modular input files and code structures will be used to allow for user-customization through standardized application programming interfaces (APIs) to the general code data structures. Solution quality enhancement will be made possible by inclusion of automated or user-controlled adaptation features in the code. These include features relating to numerical solution quality (such as grid cell size, timestep size, or statistical scatter) and physical realism (such as the complexity of the gas representation or the collision models used).

Initial interfaces to the codes will be through keyword-based text files. Later versions will utilize optional GUIs. The pre-processor will perform input file error checking, job setup, and initialize the SUPREM-DSMC data structures. The main code will be designed for batch operation on large HPC computers, but the provision will made for interactive operation. The post-processor will allow for extraction and reformatting of relatively arbitrary user-defined data for plotting and analysis.

The input files to the codes will consist of geometry, boundary condition, gas species and collision definition, and execution control. These files will be designed to provide both definition of the problem itself, and a concise documentation of the processes actually used in the code. In this way, the user can directly understand (or at least must explicitly define) what documented features, techniques, or models are being used, without recourse to the "blackbox" source code. The files will be hierarchical, such that a basic case can be easily set up, but a more experienced user can define increasingly complex models to be used, or phenomena to be resolved. The execution control file will describe the basic features of the job such as desired spatial and temporal accuracy, memory or run-time constraints.

GRIDDING

SUPREM-DSMC will use a two-level, 3-D cartesian computational grid. The Level 1 grid may be a uniform or clustered grid, and will be initialized at the beginning of the computation. As the calculation proceeds, a Level 2 adapted grid will be generated, where the adaptation criteria may be the mean free path or number density, or possibly a local flow gradient or other detailed property. The grid will be defined and stored independently of the input geometry. The geometry will be defined in terms of simple geometric primitives for simple bodies, or surface triangulations for more complex bodies. Boundary surfaces will be discretized on the Level 2 grid to facilitate the molecule movement process, whereas load balancing will be done at Level 1.

The Alpha-version of the code will model 2-D stationary geometries, where the user specifies the characteristics of the Level 2 grid and surface elements. The data structures will be sized and allocated based on a user-specified grid dimension or size, and load balancing will be static, based on the grid volume. Spatial weight factors will be constant based on an estimated value, but may be globally adjusted to satisfy memory (number of simulation particles) constraints.

The Beta-version of the code will include 3-D stationary geometry and 2-D rigid body motion. The Level 2 grid and surface elements will be automatically generated. In addition, the Beta-version will include an interface with a CAD or grid-generation program to generate the surface grid; in this case, if further grid refinement is necessary, SUPREM-DSMC will generate the appropriate 3-D surface grid by subdividing the input geometry surface triangulation as part of the grid adaptation process. Data structures will be sized and allocated based on reference flow conditions or from an existing solution. Load balance may be either static, based on estimated work or on an existing solution, or dynamic, based on CPU time. Computational cell structure will be adapted to a local bulk flow property, such as mean free path, or adapted to a local flow gradient or detailed property, while surface elements will be adapted to a near surface local flow property. Capabilities for spatial weight factors will include: a global adjustment to satisfy collision separation constraints, a local constant flux value (adjusted with timestep), a global adjustment to accelerate transient computation, or a local adjustment to obtain desired local molecule cell population.

BOUNDARY CONDITIONS

The boundary conditions are grouped into general types and sub-types to allow for a wide variety of models and processes to be simulated for the creation of, or reflection of, molecules at computational boundaries. For example, a wall reflection process can vary from a simple diffuse interaction in the Alpha version of the code to a chemical reaction process dependent on specific energy modes of the colliding species in later versions. Similarly, capabilities for the general description of inflow, outflow, and symmetry boundaries will be included. Future enhancements (possibly beyond the CHSSI project timeframe) include, for example, capabilities for 3D rigid body motion, and 2-D and 3-D generalized boundary motion.

MOVEMENT OF MOLECULES

Molecules will be moved on the Level 2 grid. Molecules will be moved in sub-iterations, where the displacement is limited, if necessary, to the boundary of the Level 2 cell in which it initially resides. This is necessary to avoid translation errors when a molecule moves across Level 2 cells with varying timesteps and to account for spatial weighting factors. Ray tracing techniques will be used to compute the potential intersection of the molecule trajectory with boundary elements. Communication buffering techniques will be used to address the movement of a molecule to a computational cell which is assigned to another processor.

The alpha-version will allow for the movement of molecules through a 2-D fixed grid and geometry. Beta-version capabilities include movement of molecules through a 2-D adapted grid and through a 3-D fixed and adapted grid. In addition, the beta-version will allow for movement of molecules through a grid with variable spatial weighting factors and timesteps, and through a 2-D grid in which there is a defined geometrical boundary motion.

GAS SPECIES, COLLISIONS AND CHEMICAL REACTIONS

The gas species representation, the collision processes they can experience, and the models used to describe the interaction will be defined in the gas species input file, rather than being hardwired internal to the code. The species definition can include an arbitrary number of continuous or quantized internal energy modes, and thus allows for representation of atomic through arbitrary polyatomic species. Each quantized internal energy mode may include a specification of one or more radiative lifetimes, and the code will allow for the effects of unimolecular (radiative) depletion of excited modes. If desired, specific quantized levels can be defined as separate "species" to improve representation via species weighting factors, or to allow rudimentary representation of state-specific processes. SUPREM-DSMC will not include coupled radiation, and it is not planned to have the code output radiance maps, but every effort will be made to make the output compatible with existing post-processor radiance codes. It is anticipated that these features will be added in follow-up work after the initial CHSSI project in completed.

The collision events are described by chemical reaction equations which define the species involved, the energy modes that contribute to, or take part in, the collision, and the models used to carry out the process. An arbitrary number of potential collision processes can be defined for a given species pair. The event selection is done using the null collision scheme, where the event probability is related to the relative magnitude of the event (i.e., approximately the event cross section), and only one event occurs per collision (but it can involve relatively arbitrary changes in the colliding species).

The collision events are nominally categorized as elastic, inelastic, or general reaction processes. Several basic DSMC models will be pre-defined for each category, but the basic approach allows for the consistent inclusion of a wide variety of processes and models to be defined and implemented by the user as they become available. For elastic collisions, the variable hard sphere[1] or variable soft sphere[7] models will be available. For inelastic processes involving the redistribution of one internal mode of one molecule, a collision number (constant probability) scheme will be provided, where an accepted event undergoes redistribution of the mode via the Borgnakke-Larsen model. The general class of reaction events allows for definition of arbitrary changes to the species and the modes involved in the collision. A generalized form of the Bird total collision energy model[1] based on known (input) Arrhenius rate coefficient data will be provided. In this form, the user may specify which internal energy modes of each reactant contribute to the reaction probability, a feature not included in some earlier versions of this model. Finally, for each of the general event categories, allowance is made for input of tabulated cross section data for cases where no analytical model of an event is available or suitable.

The present level of maturity of models of chemical and collision events in DSMC precludes definitive determination of a unique database which satisfies both computational efficiency and physical accuracy requirements for the general problem. Continuing research, both internal to and external to the

AFRL/NRL team, is expected to provide improvements in this area and any relevant results from these efforts will be utilized to the fullest extent possible during SUPREM-DSMC development. To assist the novice user, several standardized, documented gas databases will be provided with the code. The databases are expected to combine various degrees of complexity of the gas species and collision representation to allow for immediate application to specific problems involving, e.g., room temperature air, or strongly shocked atmospheric species.

PRESENT CODE STATUS

At present, code development efforts have concentrated on assembly of templates for the various modules of the software. The emphasis is on establishing consistency, generality, and extendability in the user-interface (e.g., input file definition) and for source code development (data structure representation and code modularity). The basic structure of the software is expected to be finalized by the time of the software acceptance test (SAT) scheduled for Q3 FY00.

SUMMARY AND CONCLUSIONS

A new development effort has begun that will provide the user community with a standard, scalable, parallel, reacting, multidimensional Direct Simulation Monte Carlo computational code. It is anticipated that the rocket exhaust plume community will be a major user group for SUPREM-DSMC. Potential users are encouraged to contact the developers to establish a working relationship during these early stages of development.

Though a large number of capabilities are planned for SUPREM-DSMC, the initial versions of the code will be relatively basic. The emphasis in the early phase of the project is to design the code and the user interface to present a consistent and modular new analysis capability for the greatest number of DoD users. The improved capabilities and features will be added incrementally, eliminating the need for complete rewrite of the codes, while ensuring that the time the new user invests in the initial versions will contribute to accelerated integration of the final code into his or her research, design, testing, and engineering toolkit.

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10/10/01V

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Campbell, D.H., Wadsworth, D., & VanGilder, D. (ERC); Wysong, I., Kaplan, C., & Mott, D., (Naval Research Laboratory), "SUPREM-DSMC: A New Scalable, Parallel, Reacting, Multidimensional Direct Simulation Monte Carlo Flow Code "

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